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IMPROVING THE ACCURACY OF ANGULAR-MOMENTUM PROJECTION

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SUMMARY

A connection is established between Ullah's new method of angular-momentum projection and the conventional Hill-Wheeler method. They are studied for the case where series truncation of some sort is required. It is shown that for a particular choice of angles the analysis simplifies greatly and at the same time leads to reduced truncation error.

INTRODUCTION

Recently Ullah proposed a new method (ref. 1) for performing angular-momentum projection, designed to avoid the difficulties associated with numerical integration of rapidly oscillating rotation matrices. Considering the case of axially symmetric intrinsic wave functions Φ_K, he used Löwdin's representation (ref. 2) of the projection operator P_{JK} to write

$$\Omega_J \equiv \langle \Phi_K | \Omega P_{JK} | \Phi_K \rangle$$

$$= (2J + 1) \frac{(J + K)!}{(J - K)!} \sum_{n=0}^{J_{max}-J} (-1)^n \frac{C_{J-K+n}}{n!(2J + n + 1)!} \tag{1}$$

where Ω is some rotationally invariant operator (usually H or 1) and

$$C_n = \langle \Phi_K | \Omega J_-^n J_+^n | \Phi_K \rangle \tag{2}$$

(Both Ω_J and C_n depend on K, but for simplicity this dependence will be left implicit.) Rather than evaluate equation (2) directly, Ullah showed that the coefficients C_n could be found by means of a generating function

$$\left\langle \Phi_K \middle| \Omega e^{\lambda J_-} e^{-\lambda J_+} \middle| \Phi_K \right\rangle = \sum_{n=0}^{N} (-1)^n \frac{\lambda^{2n}}{(n!)^2} C_n \qquad N \equiv J_{max} - K \tag{3}$$

and then devised an elegant transformation to reduce the left side to

$$(1 - \lambda^2)^{-K} \left\langle \Phi_K \middle| \Omega e^{-i\beta J_y} \middle| \Phi_K \right\rangle \tag{4}$$

where

$$\sin\left(\frac{1}{2}\beta\right) = \lambda$$

If equation (3) is considered for a set of $N + 1$ different values of λ, a simple matrix inversion (ref. 3) will yield the coefficients C_n.

CONNECTION WITH HARMONIC ANALYSIS METHOD

Basically, Ullah's method is an improvement of one developed previously by Mihailovic, Kuhawski, and Lesjak (ref. 4). Working from an expression which can be written (for rotationally invariant operators) in our notation as

$$\left\langle \Phi_K \middle| e^{\theta J_-} \Omega e^{\theta J_+} \middle| \Phi_K \right\rangle = \sum_{n=0}^{N} \frac{C_n'}{(n!)^2} \theta^{2n} \qquad N = J_{max} - K \tag{5}$$

they obtain the coefficients C_n' by means of harmonic analysis and then numerically solve the set of linear equations

$$C_n' = \sum_{J=K+n}^{J_{max}} \frac{(J + K + n)!(J - K)!}{(J - K - n)!(J + K)!} \Omega_J \tag{6}$$

to find the desired quantities Ω_J. This is unnecessarily cumbersome, however, since by writing

$$C'_{L-K+n} = \sum_{J=L+n}^{J_{max}} \frac{(J + L + n)!(J - K)!}{(J - L - n)!(J + K)!} \Omega_J \tag{7}$$

and using the identity

$$(2L + 1) \sum_{n=0}^{J-L} \frac{(J + L + n)!}{(J - L - n)!} \frac{(-1)^n}{n!(2L + n + 1)!} = \delta_{LJ} \tag{8}$$

we may easily solve the linear equations analytically, obtaining

$$\Omega_L = (2L + 1) \frac{(L + K)!}{(L - K)!} \sum_{n=0}^{J_{max}-L} \frac{(-1)^n}{n!(2L + n + 1)!} C'_{L-K+n} \tag{9}$$

the form proposed by Ullah. The identity (8) may be established by noting that the left side is proportional to the hypergeometric function ${}_2F_1(L + J + 1,\ L - J;\ 2L + 2;\ 1)$. This in turn may be written in closed form, and the left side reduces to $(2L + 1)/(L + J + 1)(L - J)!(J - L)!$

Another difficulty is that the transformation used by Mihailovic, Kujawski, and Lesjak to render their equations harmonic requires evaluation of equation (5) at $2N + 1$ different complex values of θ to obtain the $N + 1$ coefficients C'_n. Since calculation of the overlap integral in equation (5) is difficult and lengthy on even the fastest computers, the direct method proposed by Ullah, which requires only $N + 1$ different evaluations, is to be preferred.

There still remains a problem, however. If the dimensionality of the model space used to define Φ_K is allowed to increase, or an "inert" core is allowed to become "active", the value of J_{max} can become enormous. In that case the expansion (3) must be truncated for practical reasons, and it is not clear how to choose the set of λ values so as to minimize the truncation error.

CONNECTION WITH HILL-WHEELER METHOD

It is instructive to compare Ullah's method with the conventional one employing the Hill-Wheeler integral (ref. 5),

$$\Omega_J = \frac{2J+1}{2}\int_0^{\pi}\left\langle \Phi_K \middle| \Omega e^{-i\beta J_y} \middle| \Phi_K \right\rangle d^J_{KK}(\beta)\sin\beta\, d\beta \tag{10}$$

where

$$d^J_{KK}(\beta) \equiv \left\langle JK \middle| e^{-i\beta J_y} \middle| JK \right\rangle$$

is an element of the reduced rotation matrix. It has been pointed out by Ripka (ref. 6) that direct numerical integration of equation (10) is likely to be inaccurate for large values of J, because of the rapid oscillations of $d^J_{KK}(\beta)$. The factor $\langle \Phi_K | \Omega \exp(-i\beta J_y) | \Phi_K \rangle$, on the other hand, is relatively smooth except for a strong peak at $\beta = 0$ (and possibly at $\beta = \pi$) (refs. 7 and 8). This suggests an expansion in powers of some suitable function of β, and from Ullah's work (see eqs. (3) and (4)) it is apparent that one such expansion, with only a finite number of terms, is

$$\left\langle \Phi_K \middle| \Omega e^{-i\beta J_y} \middle| \Phi_K \right\rangle = \left(\cos\frac{1}{2}\beta\right)^{2K}\sum_{n=0}^{N}(-1)^n\frac{C_n}{(n!)^2}\left(\sin\frac{1}{2}\beta\right)^{2n} \tag{11}$$

Using equation (11) in (10) results in

$$\Omega_J = \frac{2J+1}{2}\sum_{n=0}^{N} C_n Q_n^{JK} \tag{12}$$

where

$$Q_n^{JK} = \frac{(-1)^n}{(n!)^2}\int_0^{\pi}\left(\sin\frac{1}{2}\beta\right)^{2n}\left(\cos\frac{1}{2}\beta\right)^{2K} d^J_{KK}(\beta)\sin\beta\, d\beta$$

$$= \frac{(-1)^n}{(n!)^2}\int_{-1}^{1}\left(\frac{1-x}{2}\right)^n\left(\frac{1+x}{2}\right)^{2K} P_{J-K}^{(0,2K)}(x)dx \tag{13}$$

Here the reduced rotation matrix has been replaced by its representation in terms of a Jacobi polynomial (ref. 9). Because of the orthogonality property of Jacobi polynomials, the integral in equation (13) vanishes unless $n \geq J - K$. Its nonvanishing values are given by (ref. 10)

$$Q^{JK}_{J-K+n} = 2(-1)^n \frac{(J+K)!}{(J-K)!} \frac{1}{n!(2J+n+1)!} \tag{14}$$

and we recover Ullah's result.

A SIMPLIFIED METHOD BASED ON ORTHOGONAL POLYNOMIALS

The previous section illustrates the connection between Ullah's expansion and the conventional Hill-Wheeler integral treatment. The orthogonality feature, however, suggests a different expansion of the integrand factor in equation (10), namely, that the terms in equation (11) be rearranged so that

$$\left\langle \Phi_K \middle| \Omega e^{-i\beta J_y} \middle| \Phi_K \right\rangle = \left(\cos \frac{1}{2} \beta\right)^{2K} \sum_{J=K}^{J_{max}} a_J P^{(0,2K)}_{J-K}(\cos \beta)$$

$$= \sum_{J=K}^{J_{max}} a_J \, d^J_{KK}(\beta) \tag{15}$$

We then obtain the remarkably simple result

$$\Omega_J = \langle \Phi_K | \Omega P_{JK} | \Phi_K \rangle = a_J \tag{16}$$

Of course, this is really not so surprising, since equations (10) and (15) together form a statement of the expansion theorem for orthogonal functions, that is, one implies the other. The importance of equation (15), however, is not only that its coefficients $a_J = \Omega_J$ may be obtained by exactly the same procedure suggested by Ullah, namely, matrix inversion, but in addition that for a particular choice of angles it is possible to arrange matters so that the matrix inversion can be done trivially and yet furnish a superior approximation to the integral if the expansion is truncated at $J = J_o$.

This is accomplished by using the roots β_n of the first neglected rotation matrix

$$d^{J_o+1}_{KK}(\beta_n) = 0 \qquad n = 0, 1, \ldots, N_o = J_o - K \tag{17}$$

(excluding the 2K-multiple root $\beta = \pi$), because for these angles the Christoffel-Darboux formula (ref. 11) for Jacobi polynomials yields an "orthogonality" relation:

$$\sum_{J=K}^{J_o} \left(\frac{2J+1}{2}\right) d^J_{KK}(\beta_m) d^J_{KK}(\beta_n) = 0 \qquad m \neq n \tag{18}$$

With this relation the $N_o + 1$ linear equations obtained by setting $\beta = \beta_n$ in equation (15) are easily solved, yielding

$$\Omega_J = \sum_{n=0}^{N_o} W_n \left[\left(\frac{2J+1}{2}\right) d^J_{KK}(\beta_n) \left\langle \Phi_K \middle| \Omega e^{-i\beta_n J_y} \middle| \Phi_K \right\rangle\right] \tag{19}$$

where

$$W_n = \left[\sum_{J=K}^{J_o} \left(\frac{2J+1}{2}\right) d^J_{KK}(\beta_n)^2\right]^{-1} \tag{20}$$

Since the Christoffel-Darboux formula is of the form

$$\sum_n^N C_n P_n(x) P_n(y) = \frac{F_n(x, y)}{y - x}$$

it follows that if $y = x + \epsilon$ with $\epsilon \rightarrow 0$, then

$$\sum_n^N C_n P_n(x)^2 = \left.\frac{\partial F_N}{\partial y}\right|_{y=x}$$

This may be used to sum the series in equation (20), with the result

$$W_n = 2\left[\frac{(J_o + 1)\sin \beta_n}{(J_o + 1 + K)(J_o + 1 - K) d^{J_o}_{KK}(\beta_n)}\right]^2 \tag{21}$$

These formulas have the appearance of an algorithm for the numerical integration of equation (10) and in fact are identical to those which would be obtained from a Gauss quadrature method of order N_o based on the orthogonal functions $d^J_{KK}(\beta)$. As such, they are known to be exact if the integrand can be expressed in terms of the first $2N_o + 1$ such functions. We conclude that, if the expansion (15) is terminated at $J = J_o$ and its coefficients are determined by equation (19), truncation error will affect <u>only</u> those Ω_J for which $J > 2J_o + 1 - J_{max}$; those with $J \leq 2J_o + 1 - J_{max}$ will remain exact. The magnitude of the truncation error is difficult to estimate, but the Gauss method is known to be remarkably accurate.

CONCLUDING REMARK

One caveat should be sounded: if the dimensionality or number of nucleons is large, the number of terms which can be taken is severely limited by the computing time required to evaluate $\langle \Phi_K | \Omega \exp(-i\beta J_y) | \Omega_K \rangle$. At the same time, the behavior of the integrand places a greater burden of accuracy on the series expansion. In a typical calculation for ^{20}Ne, for instance, with all nucleons active and states up to $1g_{9/2}$ included, the left side of equation (15) falls from 1.00 at $\beta = 0^o$ to 0.070 at $\beta = 45^o$ to 0.001 at $\beta = 65^o$. Here the strong forward peaking is of more concern than oscillations of $d^J_{KK}(\beta)$, and it may be profitable to consider a transformation on the variable of integration before attempting numerical procedures. In that event it would probable be best to treat the transformed integrand by means of a Gauss quadrature based on Chevyshev polynomials, because of the ease in calculating weights and abscissas.

Lewis Research Center,
National Aeronautics and Space Administration,
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503-10.

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